



chain nodes :

17 18 19 20 21 23 24 25 26 27 28 29 30 31 32 33 34 35

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 22

chain bonds :

1-18 2-17 3-23 5-20 6-19 9-21 11-28 12-27 14-27 15-24 20-22 21-29 23-35 24-25
24-26 29-30 30-31 31-32 32-33 32-34

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-16 13-22 14-15 14-22
15-16

exact/norm bonds :

1-2 1-6 1-18 2-3 2-17 3-4 4-5 5-6 5-20 6-19 9-21 13-16 13-22 14-15 14-22 15-16
20-22 21-29 23-35 30-31 31-32 32-33 32-34

exact bonds :

3-23 11-28 12-27 14-27 15-24 24-25 24-26 29-30

normalized bonds :

7-8 7-12 8-9 9-10 10-11 11-12

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS
22:Atom 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS
31:CLASS 32:CLASS 33:CLASS 34:CLASS 35:CLASS